

Toluene  
108-88-3 | DTXSID7021360

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 87.4 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.12e-01

Confidence level: 6.34e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Toluene</div> <div>Measured: 117</div> <div>Predicted: 87.4</div>	<div>Image not found</div> <div>Phenol</div> <div>Measured: 26.9</div> <div>Predicted: 57.3</div>	<div>Image not found</div> <div>Resorcinol</div> <div>Measured: 9.55</div> <div>Predicted: 28.3</div>
<div>Image not found</div> <div>m-Xylene</div> <div>Measured: 178</div> <div>Predicted: 246</div>	<div>Image not found</div> <div>p-Cresol</div> <div>Measured: 501</div> <div>Predicted: 95.9</div>	